Supporting Information

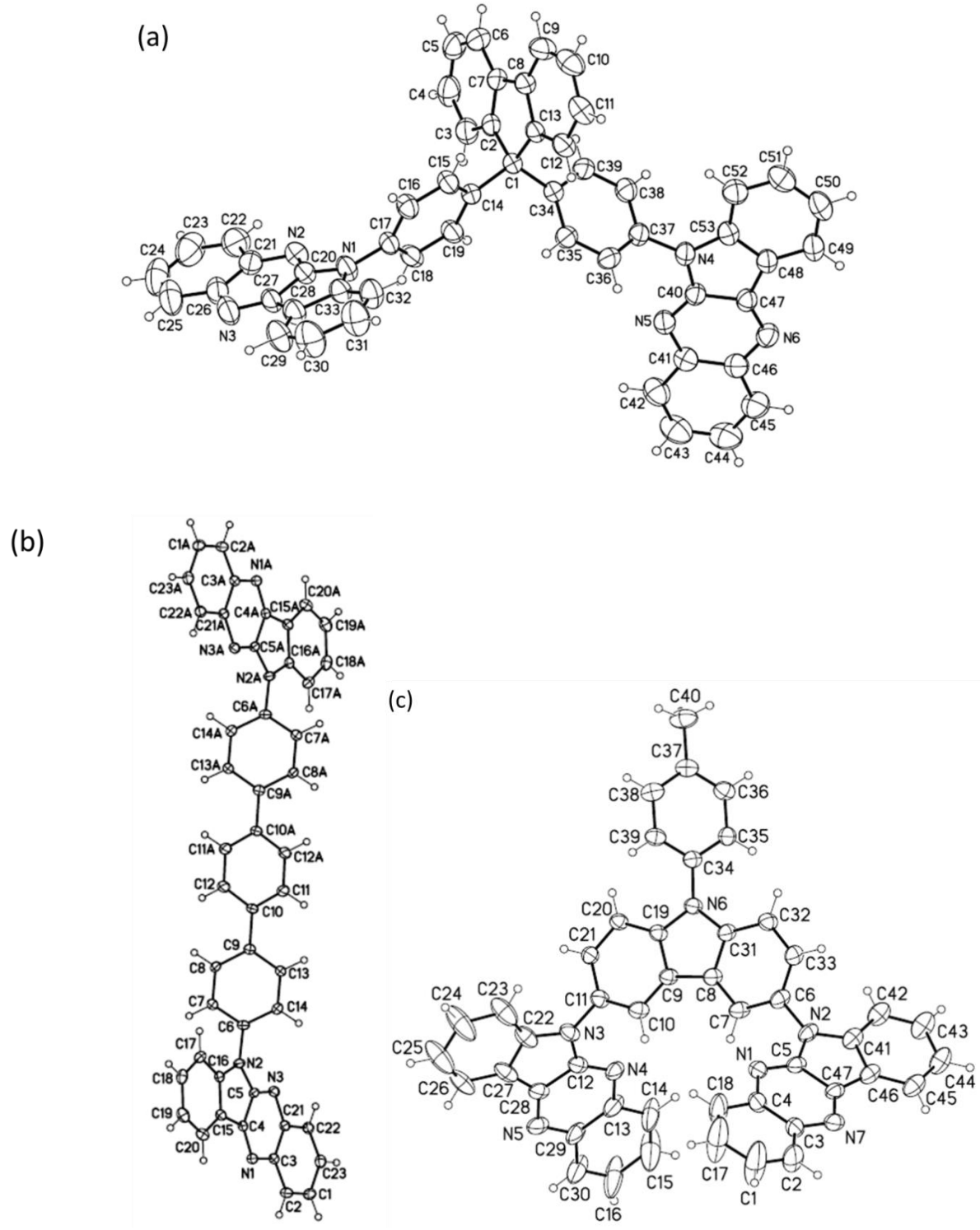


Figure S1. ORTEP drawings of (a)BIQF, (b)BIQTP and (c) BIQMCz with thermal ellipsoids shown at the 50% probability levels.

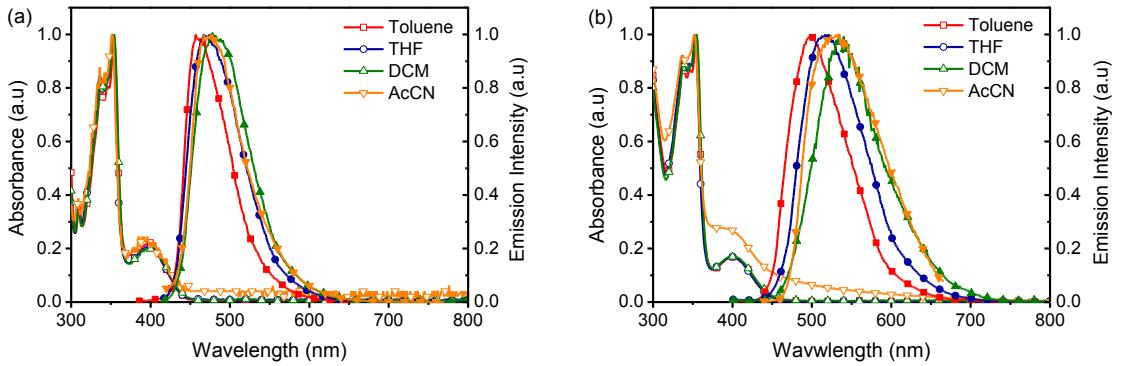


Figure S2. Optical spectra of (a) BIQF and (b) BIQMCz measured at room temperature in toluene, tetrahydrofuran, dichloromethane, and acetonitrile (10^{-5} M).

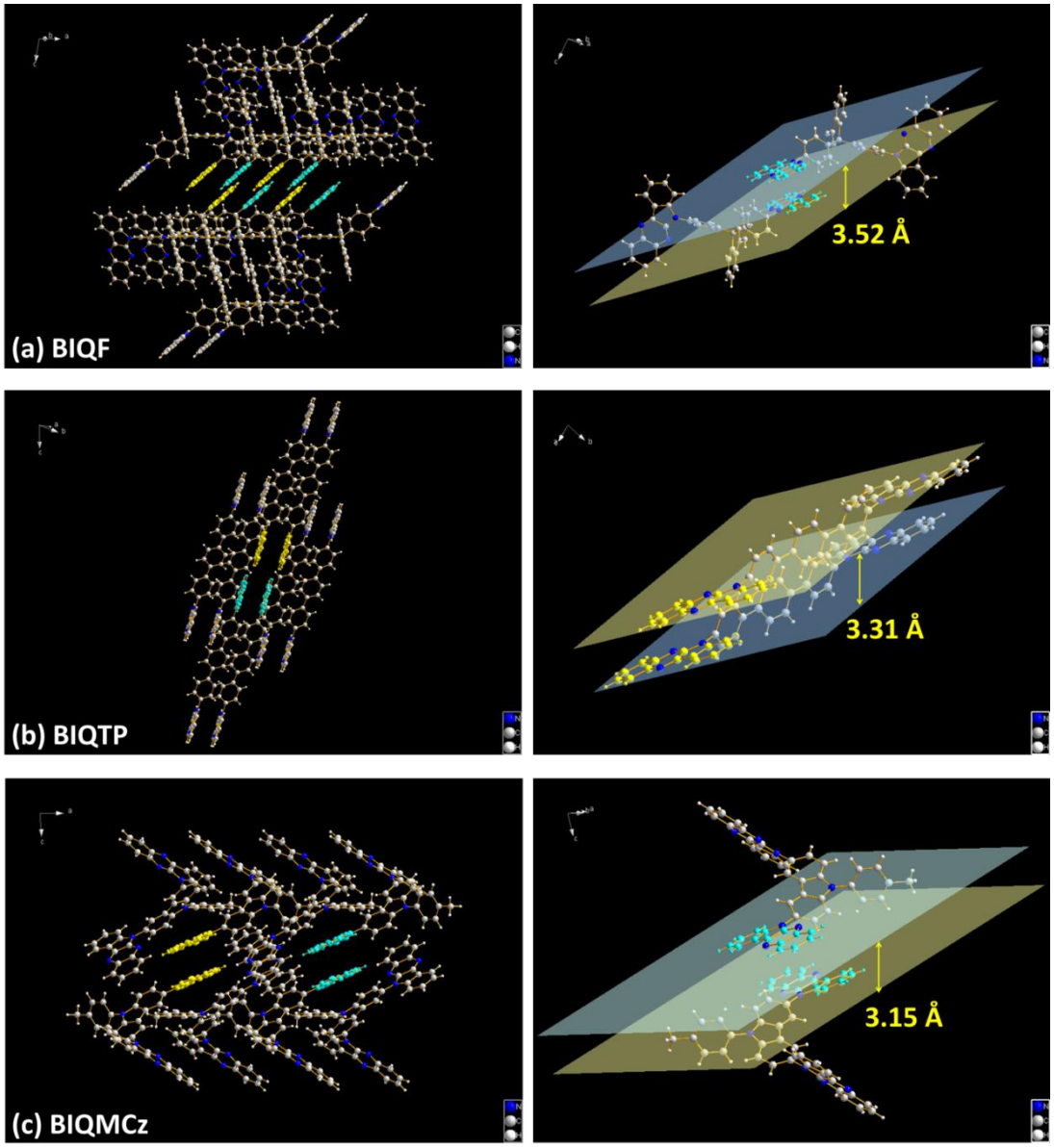


Figure S3. The molecular alignments (left, the offset stacking indoloquinoxaline moieties were depicted in the same color) and the distance between two neighboring indoloquinoxalines (right) in the crystal structure of (a) BIQF, (b) BIQTP and (c) BIQMCz.

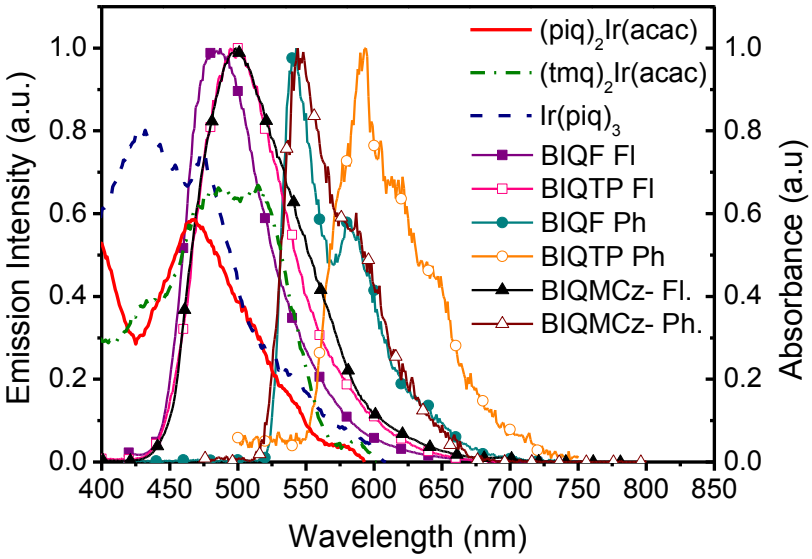


Figure S4. The fluorescence (Fl.) spectra and the phosphorescence (Ph.) spectrum of BIQF, BIQTP and BIQMCz films and excitation (intensity at 620 nm) spectra of $Ir(piq)_2(acac)$, $Ir(piq)_3$ and $Ir(tmq)_2(acac)$ measured at room temperature in dichloromethane (10^{-5} M).

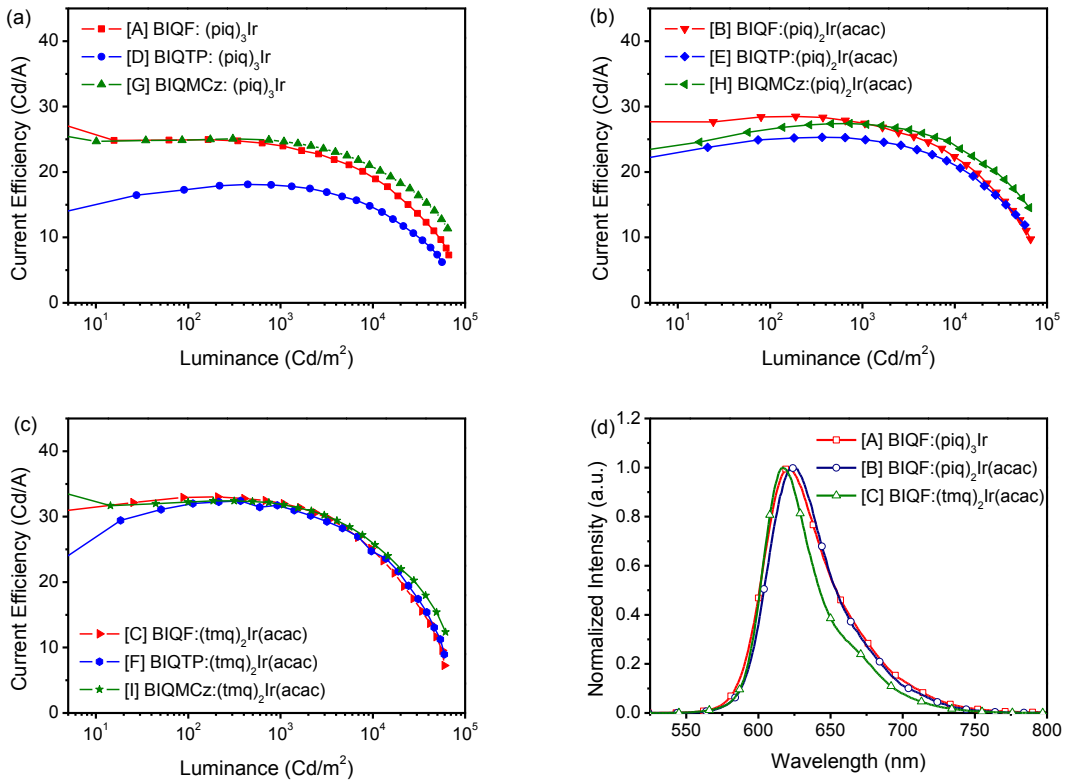


Figure S5. Current efficiency versus luminance for devices A–I, classified by dopants (a) $Ir(piq)_3$, (b) $Ir(piq)_2(acac)$ and (c) $(tmq)_2Ir(acac)$. (d) EL spectra of devices A, B and C.

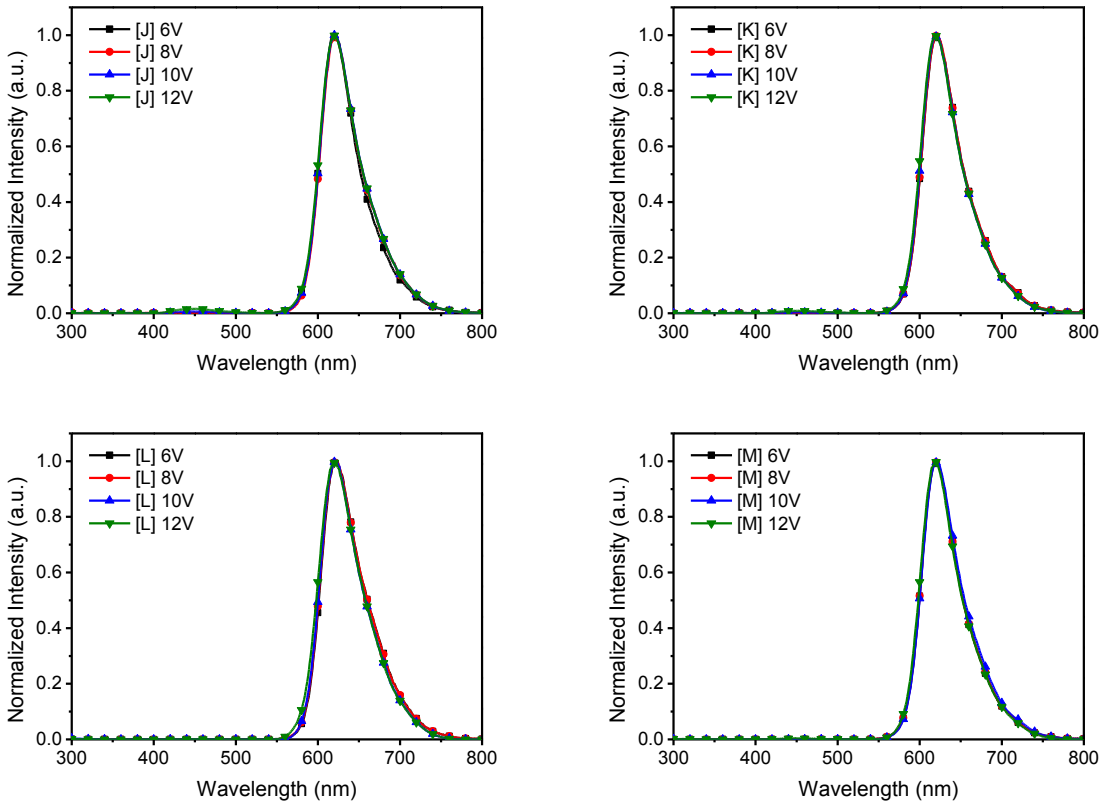


Fig.S6 The electroluminance spectra of Devices J, K, L and M at different applied voltages.

Table S1. Main excitation energies and electron contour plots of molecular orbitals of BIQF.

BIQF				
transition	most related orbitals	E_{cal}[a] (eV)	λ_{cal}[b] (nm)	f[c]
$S_0 \rightarrow S_2$	HOMO-1→LUMO HOMO→LUMO+1	3.0930	400.85	0.0258
$S_0 \rightarrow S_9$	HOMO-4→LUMO+1 HOMO-3→LUMO	3.8123	325.22	0.2860
$S_0 \rightarrow S_{10}$	HOMO-4→LUMO HOMO-3→LUMO+1	3.8206	324.51	0.2283

a. Excitation energy; b. Excitation wavelength; c. Oscillator strength.

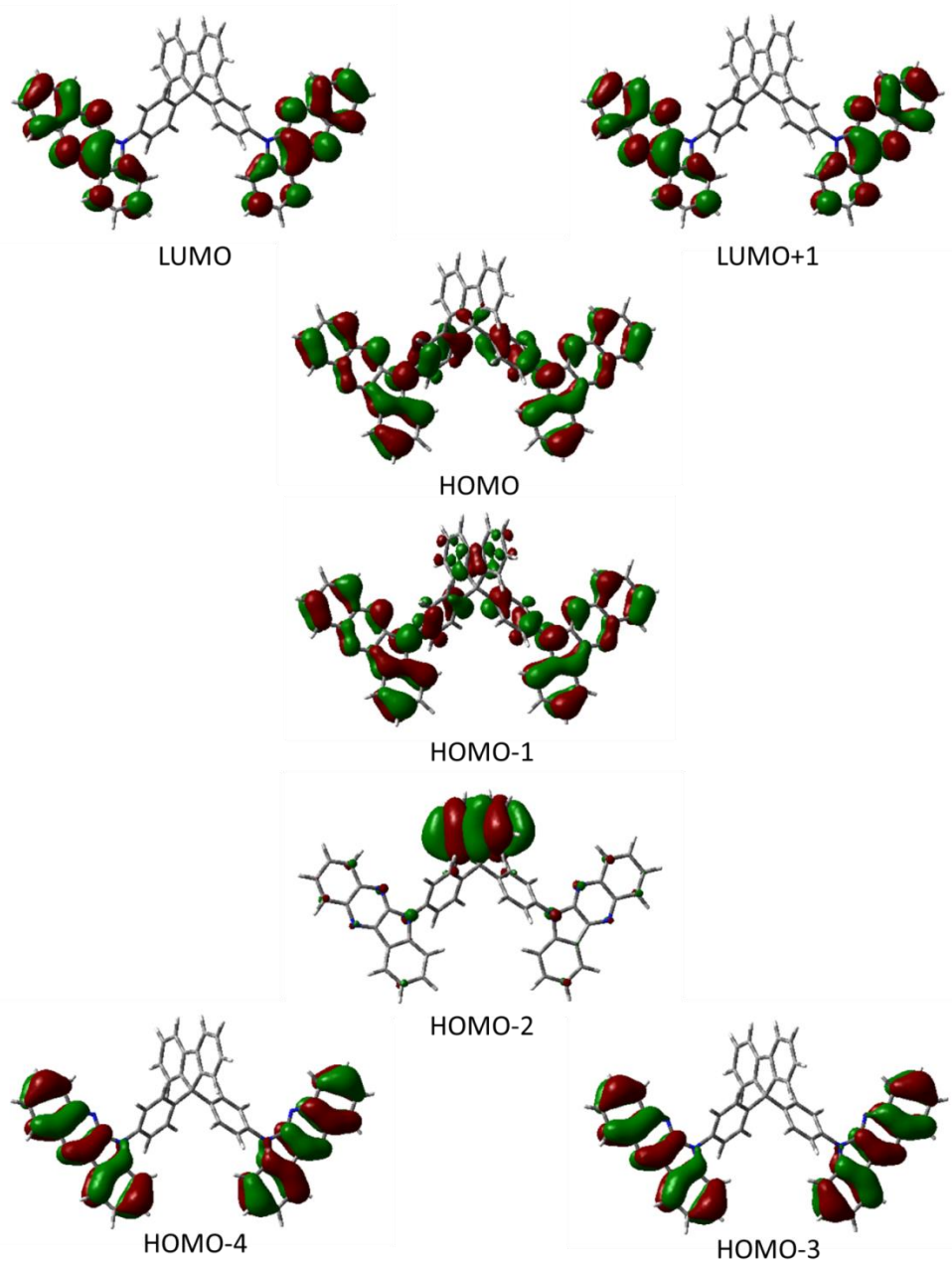


Table S2. Main excitation energies and electron contour plots of molecular orbitals of BIQTP.

BIQTP				
transition	most related orbitals	E_{cal}[a] (eV)	λ_{cal}[b] (nm)	f[c]
$S_0 \rightarrow S_1$	HOMO-1→LUMO HOMO→LUMO+1	3.0472	406.88	0.0185
$S_0 \rightarrow S_4$	HOMO-1→LUMO HOMO→LUMO+1	3.4529	359.08	0.0356

a. Excitation energy; b. Excitation wavelength; c. Oscillator strength.

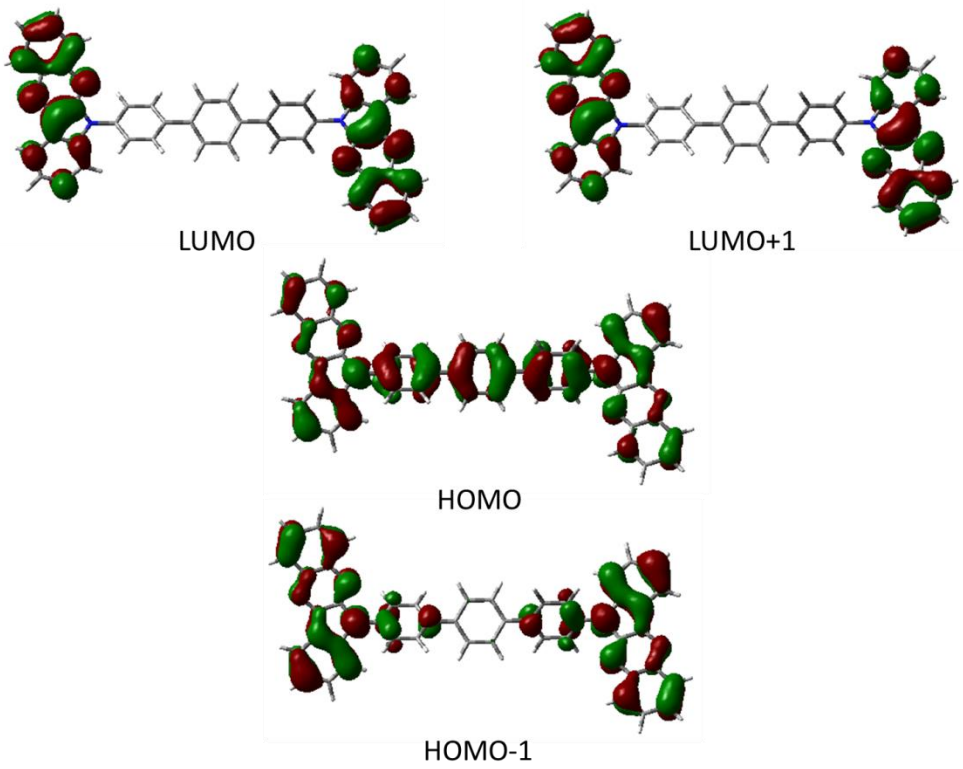
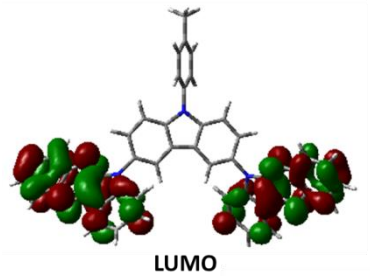
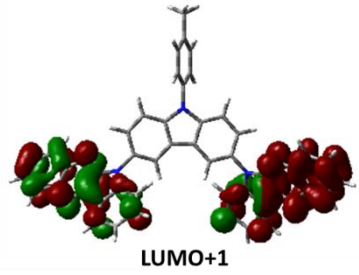


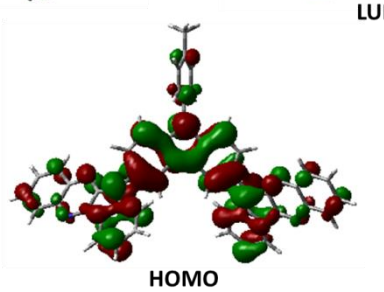
Table S3. Excitation energies and electron contour plots of molecular orbitals of BIQMCz.

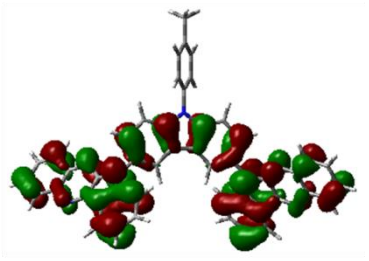
BIQMCz				
transition	most related orbitals	E_{cal}[a] (eV)	λ_{cal}[b] (nm)	f[c]
$S_0 \rightarrow S_1$	HOMO→LUMO	2.9611	418.71	0.0112
$S_0 \rightarrow S_2$	HOMO→LUMO+1	2.9623	418.54	0.0089
$S_0 \rightarrow S_8$	HOMO-2→LUMO HOMO-3→LUMO+1	3.7473	330.86	0.1230

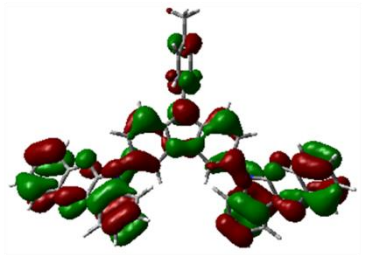
a. Excitation energy; b. Excitation wavelength; c. Oscillator strength.

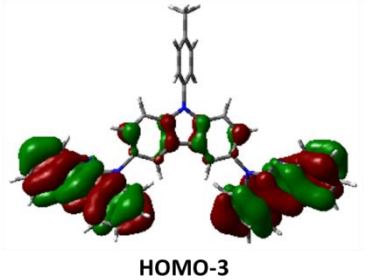

LUMO


LUMO+1


HOMO


HOMO-1


HOMO-2


HOMO-3